



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 1ISX / pdb_00001isx
Title : Crystal structure of xylanase from *Streptomyces olivaceoviridis* E-86 complexed with xylotriase
Authors : Fujimoto, Z.; Kuno, A.; Kaneko, S.; Kobayashi, H.; Kusakabe, I.; Mizuno, H.
Deposited on : 2001-12-27
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

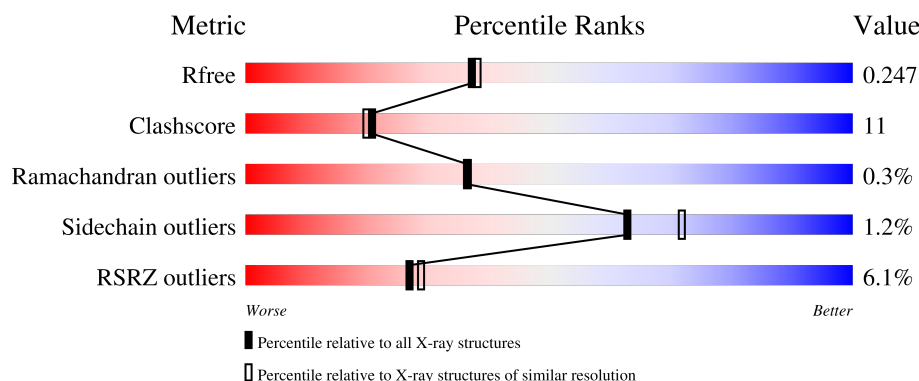
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	4% 76% 22% .
1	B	436	8% 79% 20% .
2	C	3	100%
2	F	3	100%
2	G	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	2	 50%50%
3	E	2	 50%50%
3	H	2	 50%50%

2 Entry composition [i](#)

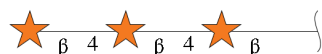
There are 5 unique types of molecules in this entry. The entry contains 7562 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called endo-1,4-beta-D-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	4	0
			3298	2025	600	656	17			
1	B	436	Total	C	N	O	S	0	4	0
			3297	2024	599	657	17			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			28	15	13			
2	F	3	Total	C	O	0	0	0
			28	15	13			
2	G	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



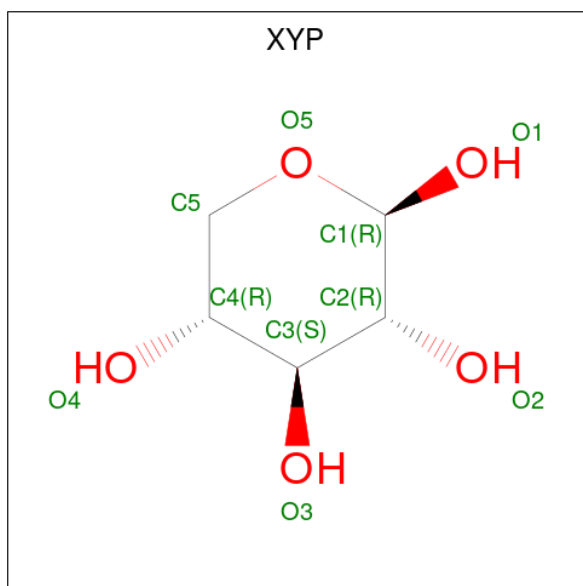
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			19	10	9			
3	E	2	Total	C	O	0	0	0
			19	10	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅).

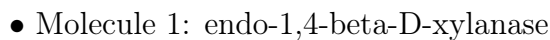


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

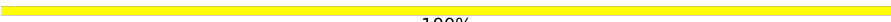
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	398	Total	O	0	0
			398	398		
5	B	408	Total	O	0	0
			408	408		

- Molecule 1: endo-1,4-beta-D-xylanase

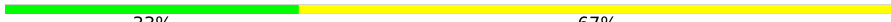


- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain F:  100%

XYP1
XYP2
XYP3

- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain G:  33% 67%

XYP1
XYP2
XYP3

- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D:  50% 50%

XYP1
XYP2

- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E:  50% 50%

XYP1
XYP2

- Molecule 3: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain H:  50% 50%

XYP1
XYP2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.37Å 94.46Å 138.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.10 29.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.82-2.10) 88.2 (29.82-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.55 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.240 0.202 , 0.247	Depositor DCC
R_{free} test set	5938 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7562	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3389	0.94	21/4599 (0.5%)
1	B	0.36	0/3388	0.91	15/4597 (0.3%)
All	All	0.36	0/6777	0.92	36/9196 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	LEU	N-CA-C	8.51	122.15	111.69
1	A	83	LEU	N-CA-C	8.46	122.10	111.69
1	B	735	THR	N-CA-C	7.92	123.05	113.23
1	A	235	THR	N-CA-C	7.56	122.96	112.45
1	A	212	SER	CA-C-N	7.44	127.44	119.78
1	A	212	SER	C-N-CA	7.44	127.44	119.78
1	B	553	GLU	CA-C-N	7.19	127.52	119.32
1	B	553	GLU	C-N-CA	7.19	127.52	119.32
1	B	537	GLU	N-CA-C	6.61	121.43	113.23
1	A	237	LEU	N-CA-C	6.44	119.69	110.10
1	A	37	GLU	N-CA-C	6.18	121.00	112.90
1	B	546	GLU	N-CA-C	6.11	119.83	112.38
1	B	866	LEU	N-CA-C	-6.04	100.96	109.96
1	B	737	LEU	N-CA-C	6.04	119.09	110.10
1	B	712	SER	CA-C-N	5.83	125.80	120.03
1	B	712	SER	C-N-CA	5.83	125.80	120.03
1	A	201[A]	CYS	N-CA-C	5.80	118.09	108.99
1	A	201[B]	CYS	N-CA-C	5.80	118.09	108.99
1	A	366	LEU	N-CA-C	-5.79	101.34	109.96
1	B	577	GLN	N-CA-C	-5.79	103.06	110.53
1	A	323	CYS	N-CA-C	5.77	119.49	110.32
1	A	407	LEU	N-CA-C	-5.68	101.87	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLU	N-CA-C	5.55	119.15	112.38
1	A	53	GLU	CA-C-N	5.54	125.21	119.56
1	A	53	GLU	C-N-CA	5.54	125.21	119.56
1	A	49	ILE	N-CA-C	5.53	115.98	110.23
1	B	669	TYR	N-CA-C	-5.49	99.78	108.73
1	A	120	ILE	N-CA-C	5.41	115.64	107.80
1	A	404	GLY	N-CA-C	-5.36	107.86	115.30
1	B	620	ILE	N-CA-C	5.33	115.63	108.17
1	A	321	GLY	N-CA-C	-5.29	107.95	115.30
1	A	169	TYR	N-CA-C	-5.27	99.94	108.52
1	B	549	ILE	N-CA-C	5.22	115.84	110.36
1	B	646	THR	N-CA-C	-5.11	106.56	112.89
1	A	77	GLN	N-CA-C	-5.08	103.97	110.53
1	A	274	TRP	N-CA-C	-5.07	106.93	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3298	0	3104	75	0
1	B	3297	0	3098	64	0
2	C	28	0	0	4	0
2	F	28	0	0	5	0
2	G	28	0	0	3	0
3	D	19	0	0	2	0
3	E	19	0	0	0	0
3	H	19	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	398	0	0	8	0
5	B	408	0	0	7	0
All	All	7562	0	6202	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139[A]:ARG:HE	1:A:140:ASP:H	1.07	0.99
1:A:1:ALA:HB1	1:A:7:ALA:HB1	1.47	0.97
1:A:139[A]:ARG:HE	1:A:140:ASP:N	1.72	0.87
1:B:822:ARG:HH12	1:B:916:ASN:N	1.84	0.75
1:B:899:VAL:HG22	1:B:906:CYS:SG	2.26	0.74
1:A:139[A]:ARG:NE	1:A:140:ASP:H	1.86	0.71
1:B:813:GLY:H	1:B:849:GLN:NE2	1.89	0.70
1:B:719:ARG:O	1:B:723:GLN:HG3	1.92	0.69
1:B:501:ALA:HB3	1:B:507:ALA:HB1	1.72	0.69
1:A:144:GLN:HE22	1:A:148:ASN:HA	1.57	0.69
1:B:822:ARG:HG2	1:B:822:ARG:HH11	1.60	0.67
1:B:705:GLN:OE1	2:F:1:XYP:O1	2.14	0.66
1:B:736:GLU:OE1	2:F:1:XYP:C1	2.43	0.65
1:A:1:ALA:HB3	5:A:1675:HOH:O	1.96	0.64
2:F:1:XYP:O1	2:G:3:XYP:O4	2.16	0.63
1:A:85:TRP:CE2	1:A:87:SER:HB2	2.34	0.62
1:B:836:GLN:HB2	1:B:876[A]:LYS:HE3	1.81	0.61
1:B:784[B]:ASN:HB3	5:B:1015:HOH:O	2.01	0.61
1:B:929:SER:HA	1:B:932:ARG:HE	1.66	0.61
1:A:432:ARG:HG3	1:A:432:ARG:HH11	1.65	0.60
1:B:671:ASP:HB3	1:B:674:ILE:HD13	1.83	0.60
2:F:1:XYP:C1	2:G:3:XYP:O4	2.50	0.59
1:A:395:ASP:O	1:A:432:ARG:HD2	2.03	0.59
1:B:818:VAL:HG23	1:B:929:SER:HB2	1.85	0.58
1:A:236:GLU:HG2	1:A:266:TRP:CE3	2.38	0.58
1:A:236:GLU:OE1	2:C:1:XYP:C1	2.52	0.58
2:F:1:XYP:O5	2:G:3:XYP:O4	2.21	0.58
1:B:585:TRP:CE2	1:B:587:SER:HB3	2.39	0.58
1:B:736:GLU:HG2	1:B:766:TRP:CE3	2.39	0.57
1:A:102:ARG:O	1:A:106:ILE:HG13	2.05	0.57
1:A:105:MET:CE	1:A:143:LEU:HD22	2.35	0.57
1:A:345:ALA:O	1:A:349:GLN:HG2	2.05	0.56
1:A:278:ASP:O	1:A:279:THR:C	2.48	0.56
1:A:2:GLU:HG2	5:A:1736:HOH:O	2.05	0.56
1:A:128:GLU:HA	1:A:171:ASP:CG	2.31	0.56
1:B:502:GLU:HB2	1:B:801:ASN:OD1	2.06	0.56
1:A:205:GLN:OE1	2:C:1:XYP:O1	2.24	0.55
1:B:720:THR:HG23	5:B:1370:HOH:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG22	1:A:406:CYS:SG	2.47	0.55
1:B:778:ASP:O	1:B:779:THR:C	2.49	0.55
1:A:53:GLU:HG2	1:A:92:TRP:HZ2	1.71	0.55
1:A:231:ASP:OD1	1:A:259:ARG:HG3	2.07	0.55
1:A:144:GLN:NE2	1:A:148:ASN:HA	2.22	0.55
1:A:190:ARG:O	1:A:194:GLN:HG3	2.07	0.54
1:A:432:ARG:HG3	1:A:432:ARG:NH1	2.23	0.54
1:B:816:LYS:NZ	1:B:816:LYS:HB3	2.23	0.53
1:B:869:ALA:HB3	5:B:1317:HOH:O	2.07	0.53
1:A:294:THR:OG1	1:A:391:ARG:HD2	2.08	0.53
1:A:142:ASN:O	1:A:146:THR:HG23	2.08	0.53
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.90	0.52
1:B:779:THR:N	1:B:780:PRO:HD3	2.24	0.52
1:B:873:ASN:ND2	1:B:924:SER:H	2.07	0.52
1:A:105:MET:HE1	1:A:150:TRP:CE3	2.45	0.51
1:A:425:CYS:HA	1:A:431:GLN:OE1	2.11	0.51
2:C:1:XYP:O1	3:D:2:XYP:O4	2.29	0.51
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.92	0.50
1:B:822:ARG:HG2	1:B:822:ARG:NH1	2.26	0.50
1:A:370:GLY:H	1:A:375:THR:HG21	1.75	0.50
1:A:426:SER:O	1:A:427:ASN:HB2	2.11	0.50
1:B:784[B]:ASN:ND2	1:B:790:LYS:HG2	2.27	0.49
1:B:846:THR:C	1:B:848:GLN:H	2.20	0.49
1:A:231:ASP:HA	1:A:259:ARG:HG3	1.94	0.49
1:B:613:MET:HE2	1:B:662:ASP:HB3	1.96	0.48
1:A:68:TYR:CZ	1:A:72[A]:VAL:HG21	2.48	0.48
1:A:303:GLY:HA2	5:A:1837:HOH:O	2.12	0.48
1:B:784[A]:ASN:OD1	1:B:786:ASP:OD1	2.32	0.48
1:B:739:ILE:HD13	1:B:746:THR:HG22	1.95	0.48
1:B:813:GLY:H	1:B:849:GLN:HE21	1.57	0.48
1:B:804:SER:HA	5:B:1320:HOH:O	2.13	0.48
1:B:876[A]:LYS:HG3	5:B:1317:HOH:O	2.12	0.48
1:B:819:GLY:O	1:B:914:THR:HG22	2.14	0.47
1:B:672:TYR:HB3	1:B:705:GLN:OE1	2.14	0.47
1:B:809:PRO:CG	1:B:935:ARG:HB3	2.45	0.47
1:B:798:ASN:HB3	5:B:1298:HOH:O	2.14	0.47
1:B:822:ARG:CZ	1:B:914:THR:O	2.63	0.47
1:A:113:MET:HE2	1:A:162:ASP:HB3	1.97	0.47
1:A:105:MET:HE3	1:A:143:LEU:HD22	1.95	0.46
1:A:131:SER:HB2	5:A:1806:HOH:O	2.15	0.46
1:A:190:ARG:HB3	1:A:190:ARG:NH1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:ARG:NH1	1:B:916:ASN:N	2.60	0.46
1:B:860:VAL:O	1:B:861:TYR:HB2	2.16	0.46
1:A:1:ALA:HA	5:A:1795:HOH:O	2.16	0.45
1:B:829:ALA:HA	1:B:847:ASN:CB	2.46	0.45
1:B:892:LEU:CD2	1:B:898:ILE:HG12	2.46	0.45
1:A:195:ARG:NH2	1:A:197:VAL:HG21	2.31	0.45
1:B:716:SER:C	1:B:718:PHE:H	2.25	0.45
1:B:819:GLY:CA	1:B:929:SER:HB2	2.47	0.45
1:A:293:TYR:C	1:A:293:TYR:CD1	2.95	0.45
1:A:338:GLN:OE1	1:A:417:GLY:HA2	2.17	0.45
1:B:818:VAL:HG23	1:B:819:GLY:N	2.31	0.45
1:A:85:TRP:CZ2	1:A:87:SER:HB2	2.51	0.45
1:B:736:GLU:HG2	1:B:766:TRP:CZ3	2.52	0.44
1:B:566:ARG:NH2	5:B:1109:HOH:O	2.46	0.44
1:A:291:ALA:HA	1:A:391:ARG:HG2	2.00	0.44
1:B:515:TYR:C	1:B:515:TYR:CD1	2.95	0.44
1:B:822:ARG:N	1:B:822:ARG:HD2	2.33	0.43
1:A:333:ASP:OD1	1:A:364:LYS:HE3	2.18	0.43
1:A:190:ARG:HB3	1:A:190:ARG:HH11	1.82	0.43
1:B:932:ARG:HG2	1:B:932:ARG:HH11	1.84	0.43
1:A:15:TYR:CD1	1:A:15:TYR:C	2.97	0.43
1:A:259:ARG:HB2	5:A:1547:HOH:O	2.17	0.43
1:A:329:ALA:HA	1:A:347:ASN:HB3	2.00	0.43
1:B:814:GLN:HE21	1:B:848:GLN:HB3	1.83	0.43
1:A:231:ASP:HA	1:A:259:ARG:CG	2.49	0.43
1:A:331:THR:O	1:A:364:LYS:HE2	2.19	0.43
1:B:517:GLY:HA2	1:B:538:PHE:HB3	2.00	0.43
2:C:1:XYP:O5	3:D:2:XYP:O4	2.37	0.43
1:A:127:ASN:ND2	1:A:128:GLU:HG3	2.34	0.43
1:A:337:VAL:HG23	1:A:420:ILE:HB	2.01	0.42
1:A:387:ASN:HB3	1:A:402:GLN:OE1	2.19	0.42
1:B:793:TYR:CD1	1:B:793:TYR:C	2.97	0.42
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.89	0.42
1:B:852:TYR:HA	1:B:857:GLU:O	2.18	0.42
1:B:860:VAL:O	1:B:864:LYS:HB2	2.19	0.42
1:A:279:THR:N	1:A:280:PRO:HD3	2.34	0.42
1:B:820:SER:O	1:B:822:ARG:HD2	2.19	0.42
1:A:311:GLY:HA2	1:A:351:THR:HG23	2.01	0.42
1:A:35:SER:HA	1:A:76:LYS:HE2	2.01	0.42
1:A:80:GLY:HA3	1:A:123:TRP:CE3	2.55	0.42
1:A:374:GLY:HA2	1:A:421:GLN:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:ASP:OD2	1:B:847:ASN:ND2	2.53	0.42
1:A:53:GLU:HG2	1:A:92:TRP:CZ2	2.55	0.41
1:A:127:ASN:CG	1:A:128:GLU:HG3	2.45	0.41
1:B:791:ALA:HA	1:B:891:ARG:HG2	2.02	0.41
1:A:106:ILE:HG22	1:A:110:ASN:ND2	2.35	0.41
1:A:186:TYR:CE1	1:A:228:LEU:HD11	2.56	0.41
1:A:305:SER:HB2	5:A:1845:HOH:O	2.20	0.41
1:B:893:ASN:ND2	1:B:899:VAL:HG23	2.36	0.41
1:B:518:THR:HA	1:B:765:VAL:O	2.21	0.41
1:A:19:ALA:HB2	1:A:266:TRP:CE3	2.56	0.41
1:A:100:THR:HG22	5:A:1766:HOH:O	2.20	0.41
1:A:105:MET:HE1	1:A:150:TRP:HE3	1.85	0.41
1:A:236:GLU:HG2	1:A:266:TRP:CZ3	2.55	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.97	0.41
1:B:813:GLY:N	1:B:849:GLN:NE2	2.64	0.40
1:B:837:VAL:HG23	1:B:920:ILE:HB	2.04	0.40
1:B:841:ASP:CG	1:B:916:ASN:HD21	2.29	0.40
1:B:873:ASN:HD21	1:B:924:SER:H	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/436 (100%)	418 (95%)	20 (5%)	0	100	100
1	B	438/436 (100%)	416 (95%)	19 (4%)	3 (1%)	18	15
All	All	876/872 (100%)	834 (95%)	39 (4%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	GLU
1	B	811	GLY
1	B	820	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/341 (101%)	340 (99%)	5 (1%)	59	67
1	B	345/341 (101%)	340 (99%)	5 (1%)	59	67
All	All	690/682 (101%)	680 (99%)	10 (1%)	63	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	201[A]	CYS
1	A	201[B]	CYS
1	A	259	ARG
1	A	280	PRO
1	B	601	LEU
1	B	701[A]	CYS
1	B	701[B]	CYS
1	B	780	PRO
1	B	816	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	55	GLN
1	A	170	ASN
1	A	173	ASN
1	A	194	GLN
1	A	284	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	314	GLN
1	B	673	ASN
1	B	814	GLN
1	B	843	HIS
1	B	849	GLN
1	B	893	ASN
1	B	921	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

15 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XYP	C	1	2	10,10,10	0.47	0	14,14,14	0.56	0
2	XYP	C	2	2	9,9,10	0.69	0	10,12,14	0.73	1 (10%)
2	XYP	C	3	2	9,9,10	0.67	0	10,12,14	0.74	1 (10%)
3	XYP	D	1	3	10,10,10	0.57	0	14,14,14	0.54	0
3	XYP	D	2	3	9,9,10	0.83	0	10,12,14	0.69	0
3	XYP	E	1	3	10,10,10	0.60	0	14,14,14	0.55	0
3	XYP	E	2	3	9,9,10	0.78	0	10,12,14	0.75	1 (10%)
2	XYP	F	1	2	10,10,10	0.48	0	14,14,14	0.58	0
2	XYP	F	2	2	9,9,10	0.66	0	10,12,14	0.73	1 (10%)
2	XYP	F	3	2	9,9,10	0.64	0	10,12,14	0.76	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XYP	G	1	2	10,10,10	0.60	0	14,14,14	0.55	0
2	XYP	G	2	2	9,9,10	0.64	0	10,12,14	0.86	1 (10%)
2	XYP	G	3	2	9,9,10	0.98	0	10,12,14	0.69	0
3	XYP	H	1	3	10,10,10	0.61	0	14,14,14	0.53	0
3	XYP	H	2	3	9,9,10	0.74	0	10,12,14	0.74	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
3	XYP	D	1	3	-	-	0/1/1/1
3	XYP	D	2	3	-	-	0/1/1/1
3	XYP	E	1	3	-	-	0/1/1/1
3	XYP	E	2	3	-	-	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	F	3	2	-	-	0/1/1/1
2	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	G	3	2	-	-	0/1/1/1
3	XYP	H	1	3	-	-	0/1/1/1
3	XYP	H	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	XYP	C4-C3-C2	-2.31	108.18	110.92
2	F	3	XYP	C4-C3-C2	-2.19	108.32	110.92
3	E	2	XYP	C4-C3-C2	-2.16	108.36	110.92
2	C	3	XYP	C4-C3-C2	-2.15	108.37	110.92
3	H	2	XYP	C4-C3-C2	-2.14	108.37	110.92
2	C	2	XYP	C4-C3-C2	-2.09	108.44	110.92
2	F	2	XYP	C4-C3-C2	-2.05	108.49	110.92

There are no chirality outliers.

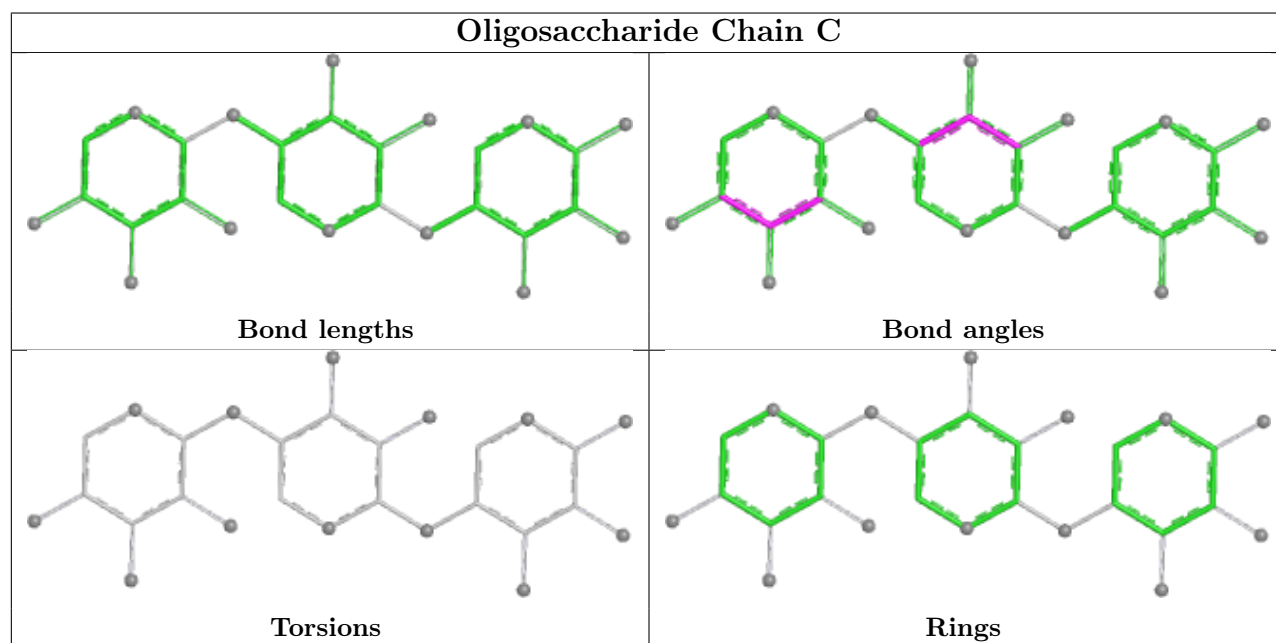
There are no torsion outliers.

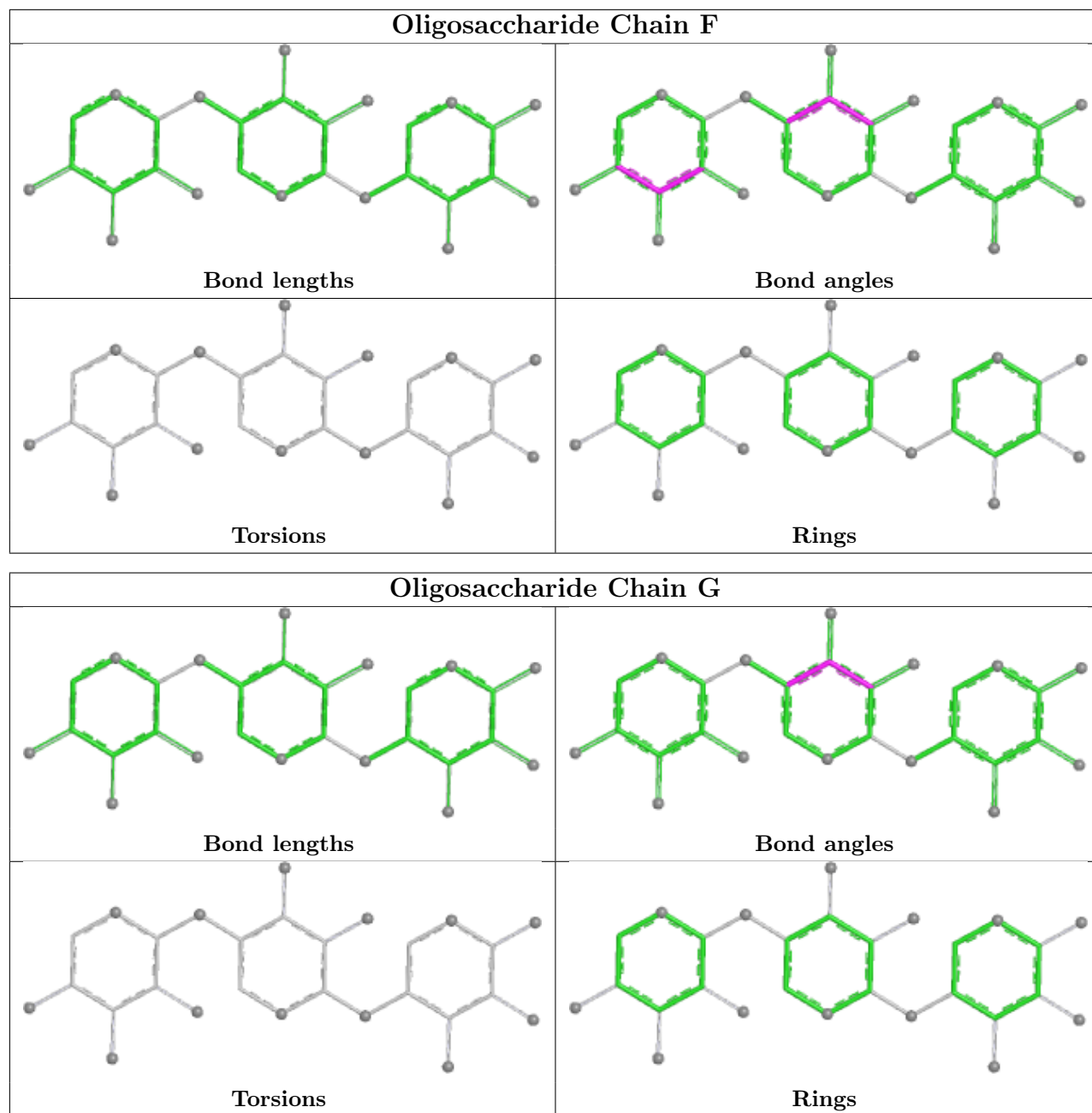
There are no ring outliers.

4 monomers are involved in 9 short contacts:

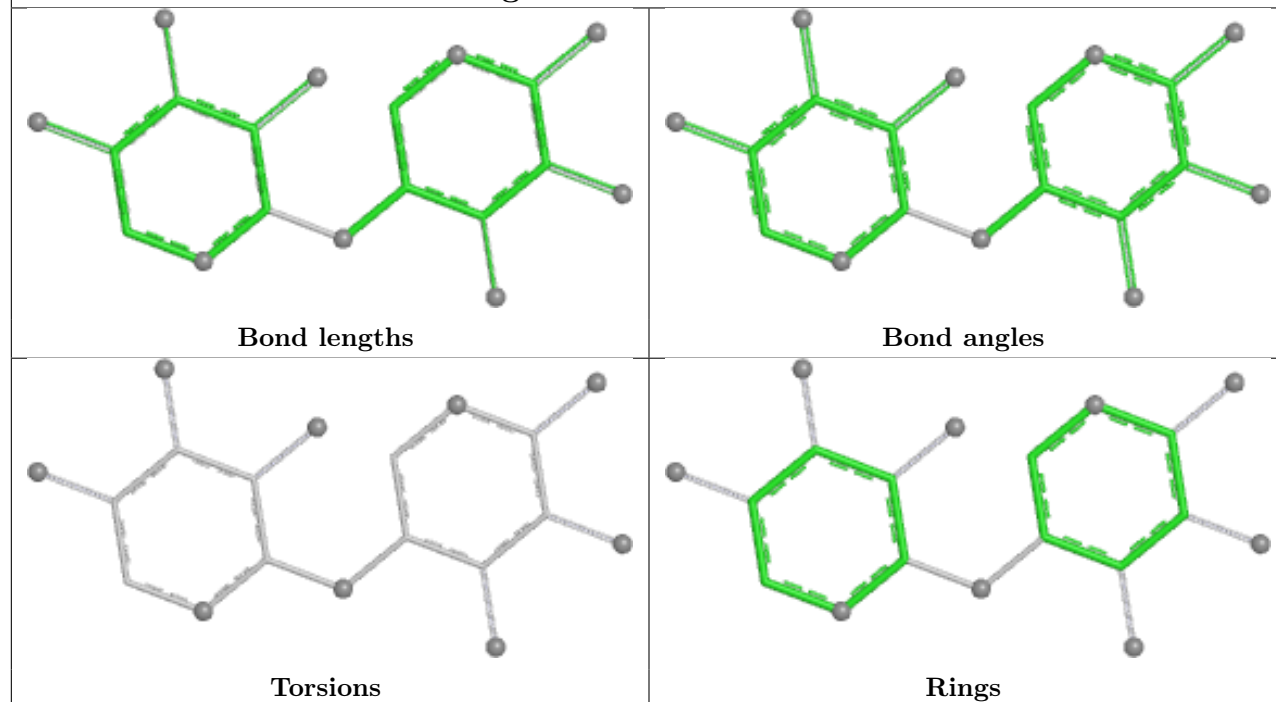
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	XYP	3	0
2	C	1	XYP	4	0
3	D	2	XYP	2	0
2	F	1	XYP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

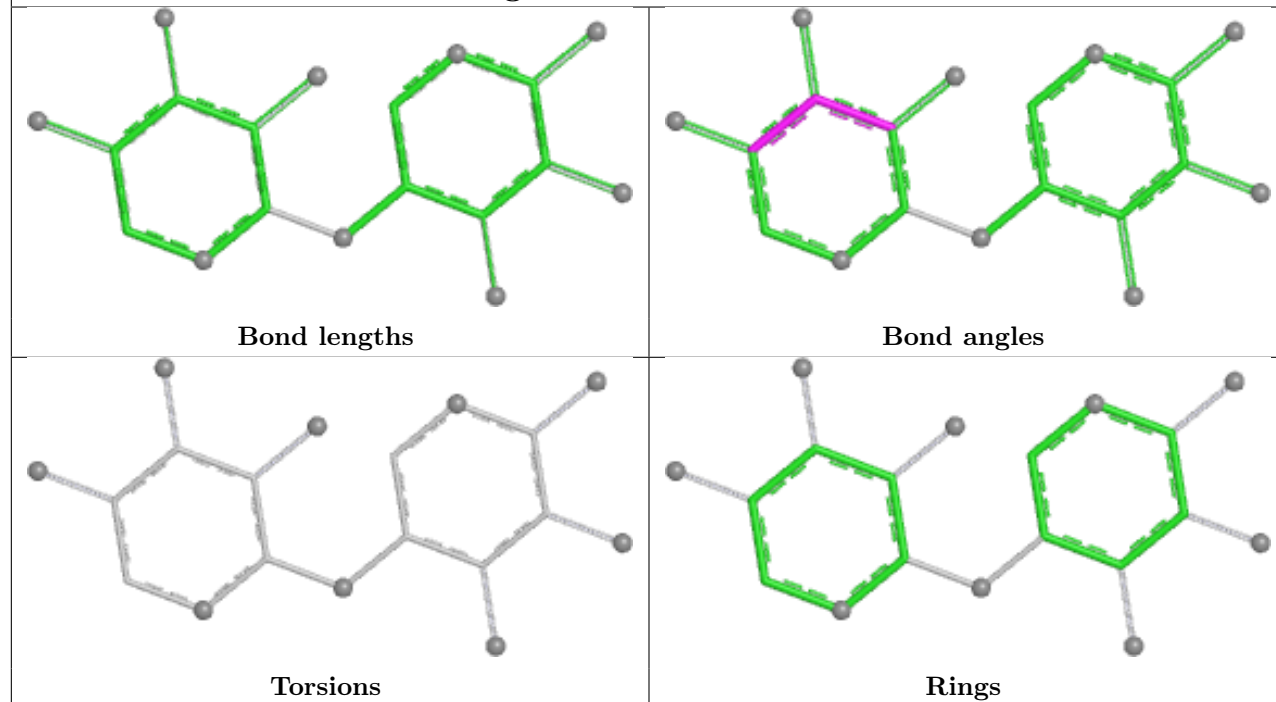


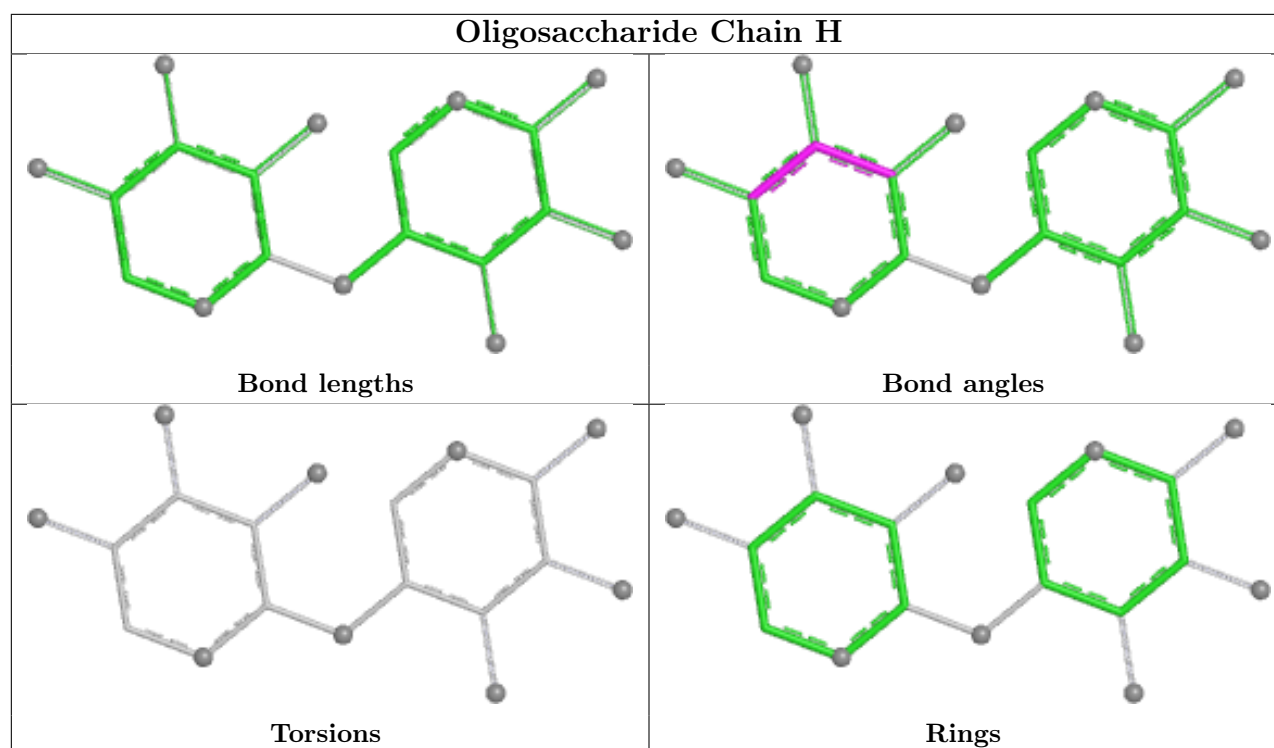


Oligosaccharide Chain D



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	XYP	B	961	-	10,10,10	0.64	0	14,14,14	0.53	0
4	XYP	A	1461	-	10,10,10	0.58	0	14,14,14	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XYP	B	961	-	-	-	0/1/1/1
4	XYP	A	1461	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	436/436 (100%)	0.01	18 (4%)	41 43	12, 22, 44, 83	3 (0%)
1	B	436/436 (100%)	0.05	35 (8%)	18 19	12, 20, 65, 76	3 (0%)
All	All	872/872 (100%)	0.03	53 (6%)	27 29	12, 21, 59, 83	6 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	THR	5.0
1	A	307	PRO	4.6
1	B	501	ALA	4.4
1	A	303	GLY	4.4
1	B	915	ALA	4.2
1	B	926	SER	3.9
1	A	2	GLU	3.9
1	B	845	ALA	3.8
1	B	840	TYR	3.7
1	A	308	PRO	3.7
1	A	309	PRO	3.7
1	B	823	CYS	3.6
1	A	304	SER	3.4
1	B	928	GLY	3.3
1	B	805	SER	3.3
1	B	818	VAL	3.3
1	A	305	SER	3.2
1	A	436	THR	3.2
1	A	311	GLY	3.1
1	B	822	ARG	3.0
1	B	815	ILE	3.0
1	A	100	THR	2.9
1	B	812	GLY	2.8
1	B	923	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	894	SER	2.7
1	A	97	SER	2.7
1	B	936	THR	2.7
1	A	139[A]	ARG	2.6
1	B	808	PRO	2.6
1	B	806	THR	2.5
1	A	312	GLY	2.5
1	B	819	GLY	2.5
1	B	846	THR	2.5
1	B	839	LEU	2.5
1	B	935	ARG	2.4
1	A	1	ALA	2.4
1	B	932	ARG	2.4
1	B	930	ASN	2.4
1	B	842	CYS	2.4
1	B	931	GLN	2.3
1	B	817	GLY	2.3
1	A	96	LEU	2.3
1	B	929	SER	2.2
1	B	809	PRO	2.2
1	B	816	LYS	2.2
1	B	918	THR	2.2
1	A	146	THR	2.2
1	B	920	ILE	2.1
1	B	814	GLN	2.1
1	B	811	GLY	2.1
1	A	66	ARG	2.1
1	B	916	ASN	2.1
1	B	555	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

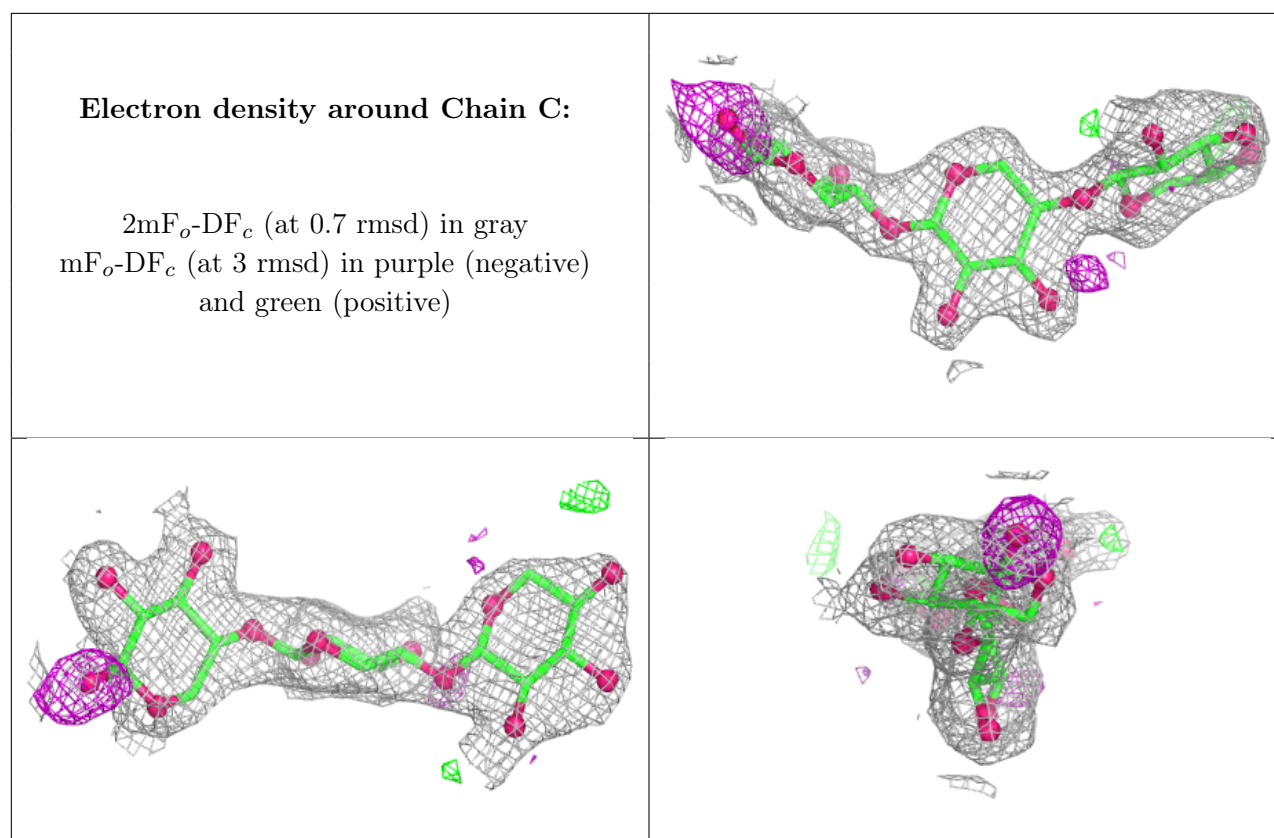
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

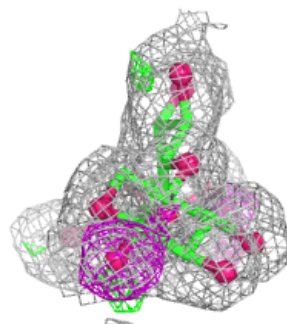
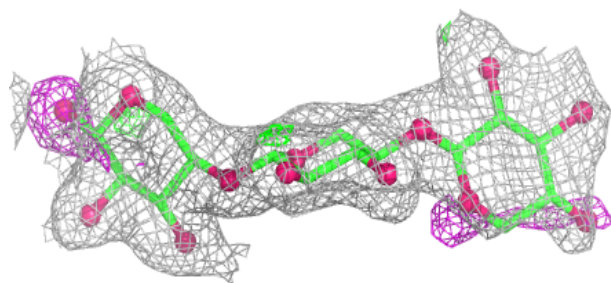
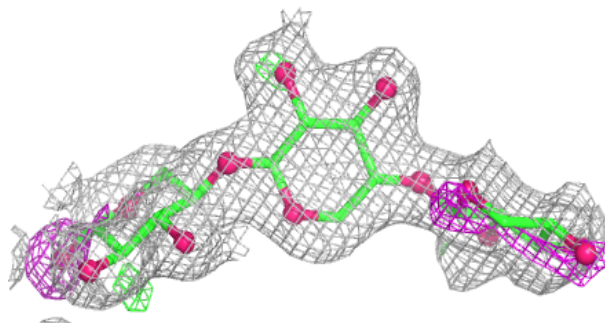
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XYP	E	1	10/10	0.72	0.16	34,42,45,48	0
3	XYP	H	2	9/10	0.74	0.13	59,60,60,60	0
3	XYP	H	1	10/10	0.76	0.14	60,61,61,62	0
3	XYP	D	2	9/10	0.79	0.16	48,50,52,52	0
2	XYP	F	3	9/10	0.79	0.15	32,36,41,42	0
2	XYP	G	3	9/10	0.81	0.13	27,29,32,32	0
3	XYP	D	1	10/10	0.81	0.17	46,48,49,50	0
2	XYP	G	1	10/10	0.83	0.16	42,48,52,52	0
2	XYP	G	2	9/10	0.84	0.14	33,34,36,37	0
2	XYP	C	1	10/10	0.85	0.12	25,28,35,40	0
2	XYP	C	3	9/10	0.88	0.10	33,36,39,40	0
2	XYP	F	1	10/10	0.89	0.10	16,19,25,35	0
3	XYP	E	2	9/10	0.90	0.10	23,24,28,29	0
2	XYP	C	2	9/10	0.93	0.07	21,23,26,28	0
2	XYP	F	2	9/10	0.95	0.07	16,16,19,24	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

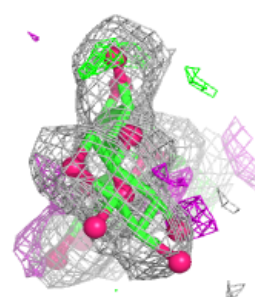
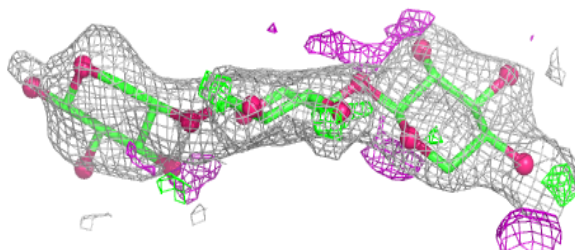
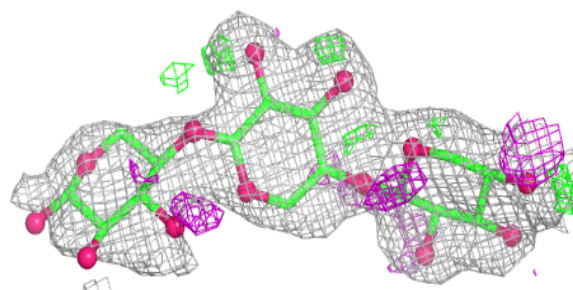


Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

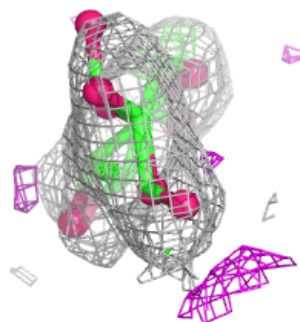
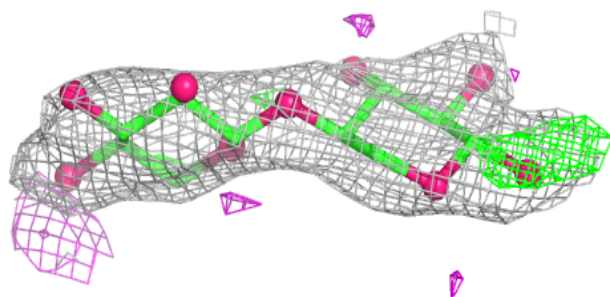
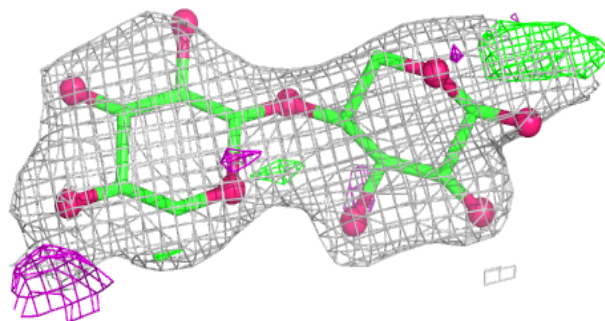
**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

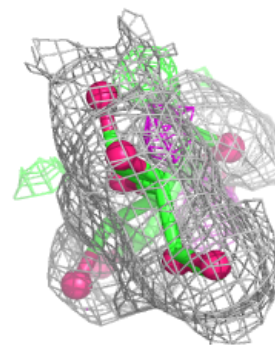
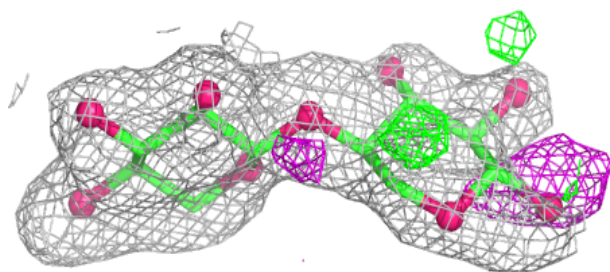
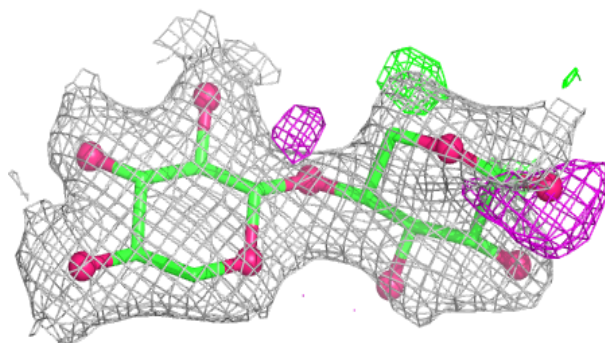


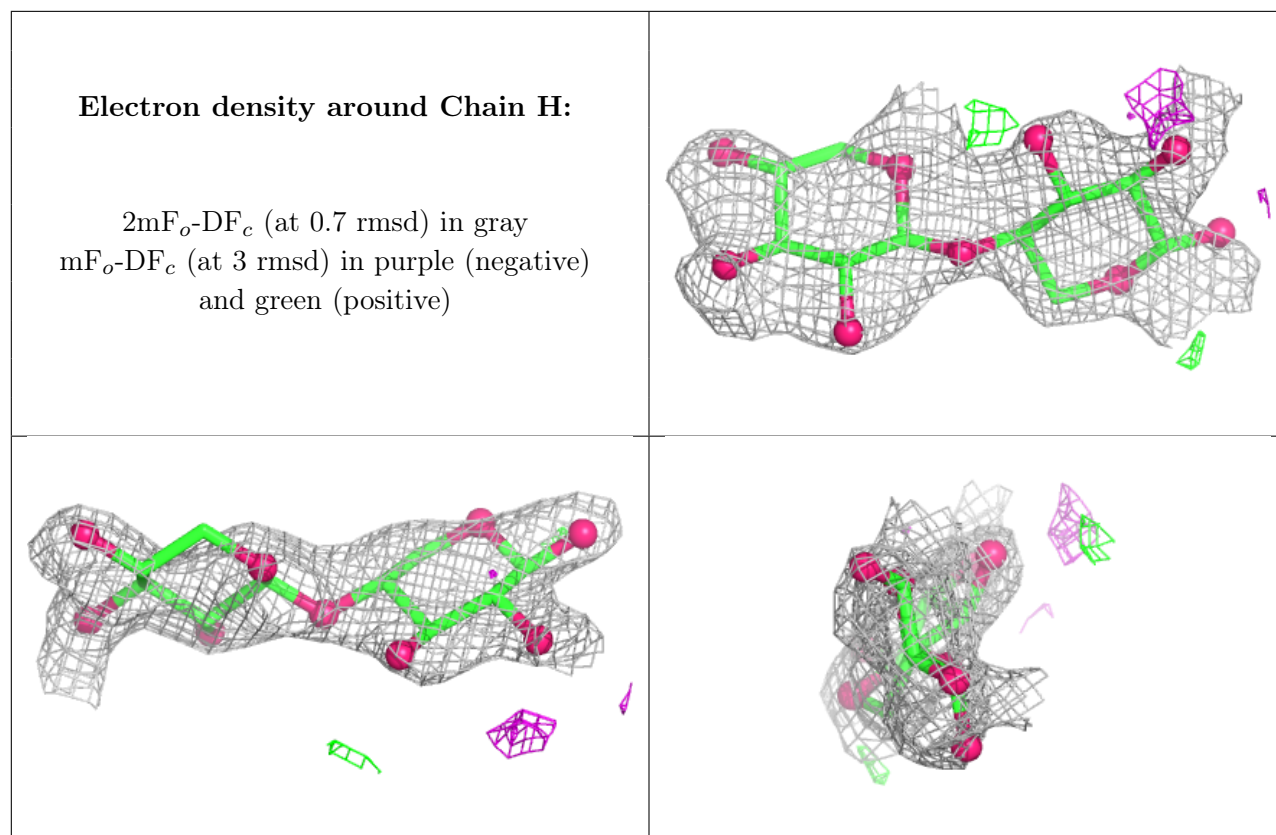
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	XYP	B	961	10/10	0.80	0.12	62,63,63,63	0
4	XYP	A	1461	10/10	0.93	0.08	29,30,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.